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Application of the generalized mean value function to the statistical detection of water in decane by near-infrared spectroscopy

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Abstract

The generalized mean value (GMV) function, defined as $G_N^{(p)} = (\Delta_N^{(p)})^{1/p}$(where $\Delta_N^{(p)}$ is the absolute value of the moment of the pth order), was used here to differentiate between statistically close random sequences or those sequences containing large numbers of measured points ($N \gg 1$). The approach taken was to find (with the help of the eigen-coordinates method) the approximate analytical function for any $G_N^{(p)}$, and in so doing demonstrate that it is inherently possible to express *quantitatively* the reduced characteristics of *any* random sequence, in terms of the 'universal' set of fitting parameters defined by this function. The introduction of a 'universal' set of the reduced parameters in the moment space then provides the instrument for the comparison of different random sequences. Applications for this new method are evident for many branches of the analytical sciences, but especially in cases when visual 'labels' (e.g. resonance lines), which serve as an indication of the presence of an additive, are either absent or 'contaminated' strongly by *noise*. Those fitting parameters from the approximate analytical expression, which depend on the concentration of the small additive can then be used for the construction of the quasi-monotonic line, defined as the *calibration curve*. Real experiments based on the treatment of near-infrared (NIR) spectra obtained for decane (the initial matrix) with water (the additive) confirm the efficiency of this simple approach. In contrast, the more conventional statistical method, based on cluster analysis, failed to establish the desired calibration curve. This simple and universal approach, which is

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